

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091818\
 Data File : BF109129.D
 Acq On : 19 Sep 2018 6:57
 Operator : JU/SJ
 Sample : J4931-04
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091418-SIDI-E-U-S

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.901	433	436	446	rVB	134626	151348	4.14%	0.635%
2	5.325	504	508	512	rBV	1354316	1215279	33.24%	5.101%
3	6.348	678	682	692	rBV	1008915	880400	24.08%	3.695%
4	6.489	701	706	709	rBV	2450486	2087021	57.08%	8.760%
5	6.719	742	745	749	rBV	979590	802354	21.95%	3.368%
6	6.878	768	772	776	rBV	3028299	2838713	77.64%	11.915%
7	7.283	835	841	844	rBV	2433688	2263634	61.91%	9.501%
8	8.001	959	963	967	rBV	1140142	896716	24.53%	3.764%
9	9.077	1142	1146	1150	rBV	3910245	3656186	100.00%	15.346%
10	9.472	1210	1213	1219	rVB	80090	70252	1.92%	0.295%
11	9.748	1257	1260	1271	rVB	942254	858784	23.49%	3.605%
12	10.536	1390	1394	1406	rBV	1414477	1374046	37.58%	5.767%
13	11.224	1508	1511	1515	rBV	866228	791272	21.64%	3.321%
14	12.813	1776	1781	1784	rBV	3781860	3626677	99.19%	15.222%
15	13.724	1929	1936	1944	rBV2	38314	71523	1.96%	0.300%
16	13.854	1954	1958	1962	rBV	1195627	1020900	27.92%	4.285%
17	14.707	2100	2103	2107	rBV	112678	101617	2.78%	0.427%
18	14.954	2142	2145	2150	rBV	43230	50501	1.38%	0.212%
19	15.259	2192	2197	2202	rBV	701835	808267	22.11%	3.393%
20	15.312	2202	2206	2210	rVB	56865	69449	1.90%	0.291%
21	15.712	2270	2274	2280	rBV	50793	73386	2.01%	0.308%
22	16.183	2349	2354	2363	rVB	42148	73616	2.01%	0.309%
23	16.730	2442	2447	2453	rVB3	22993	42942	1.17%	0.180%

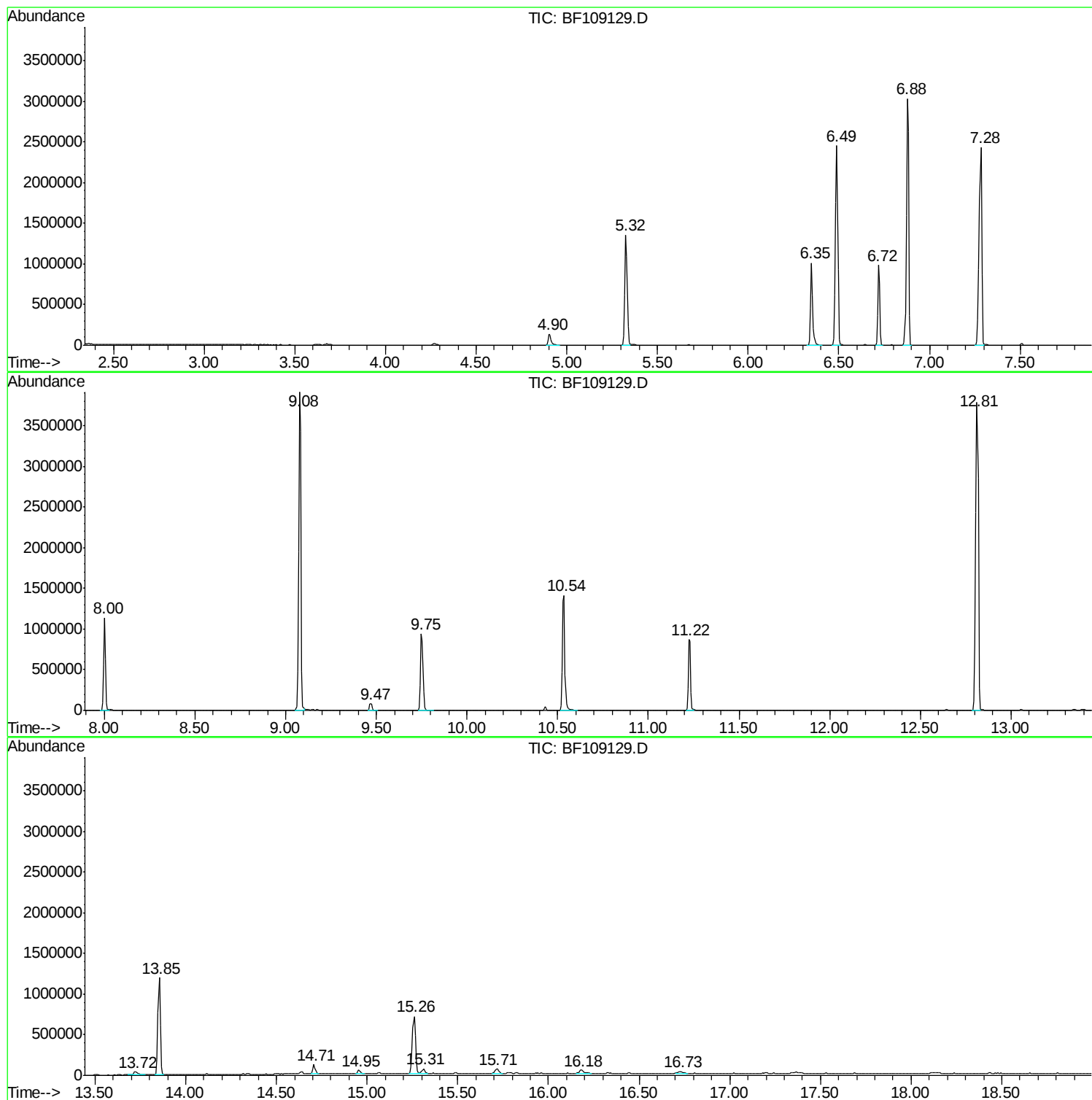
Sum of corrected areas: 23824883

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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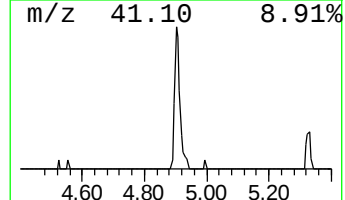
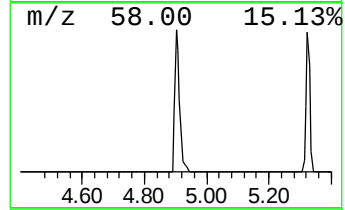
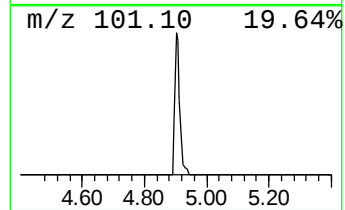
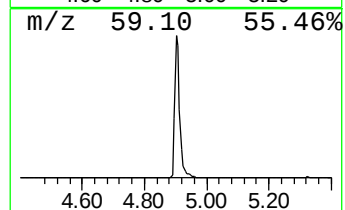
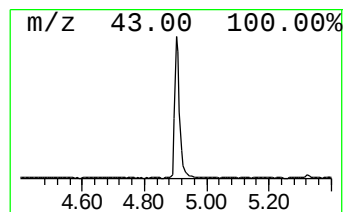
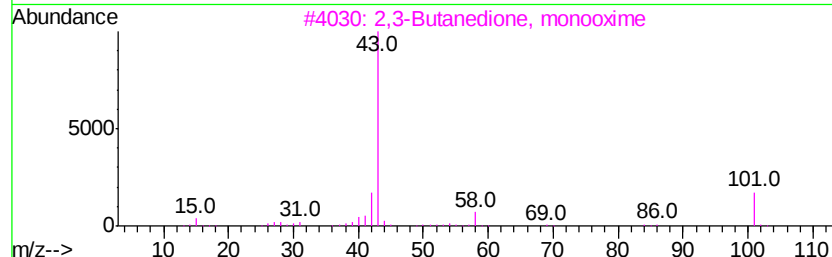
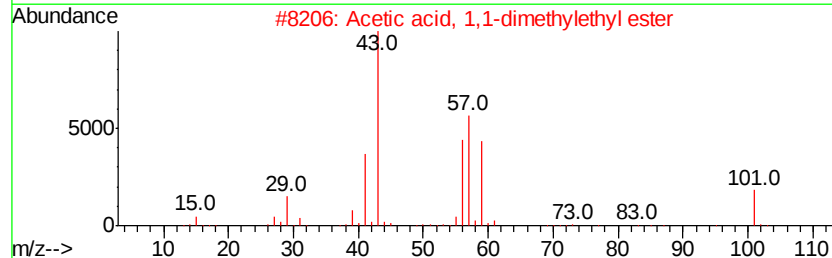
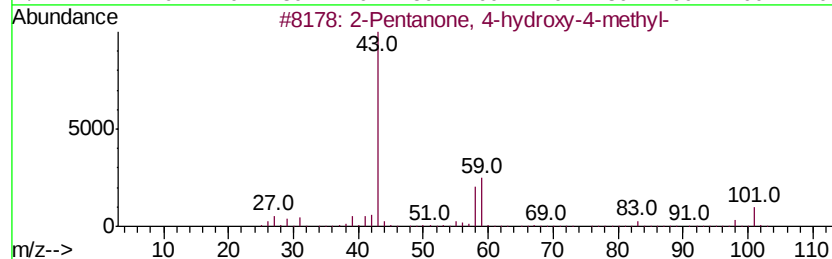
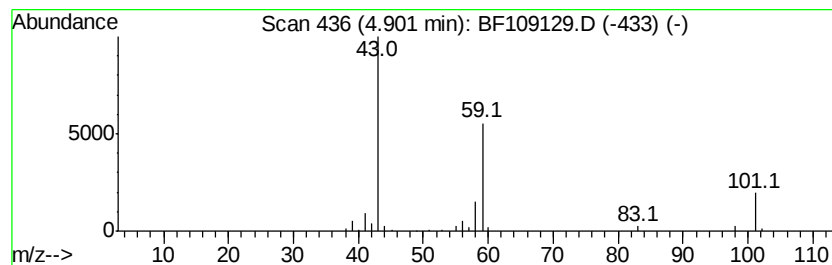
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.77 ng	151348	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol	102	C6H14O	000623-37-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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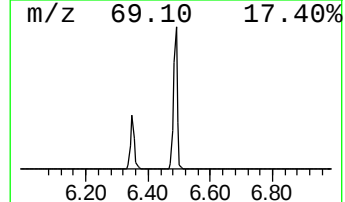
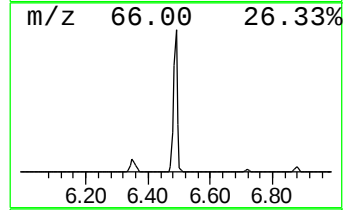
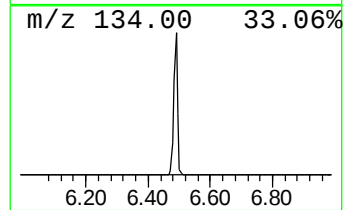
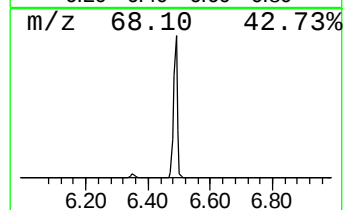
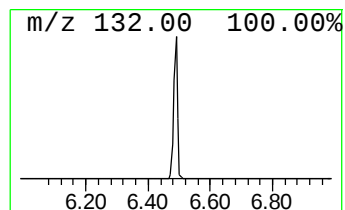
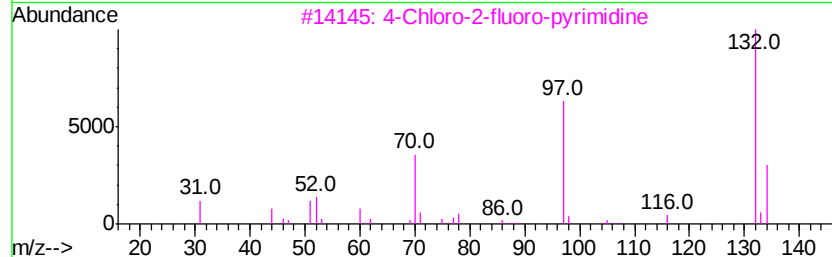
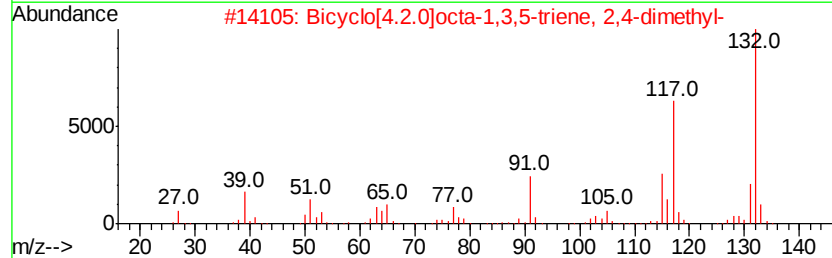
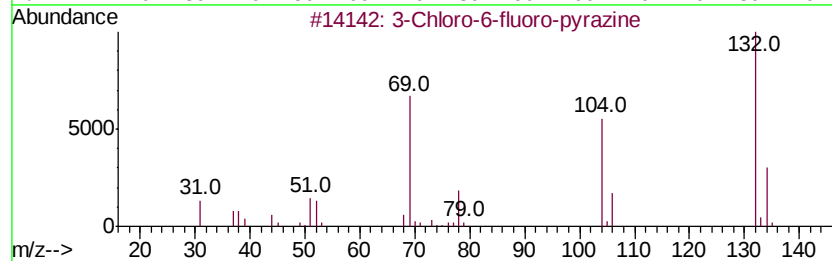
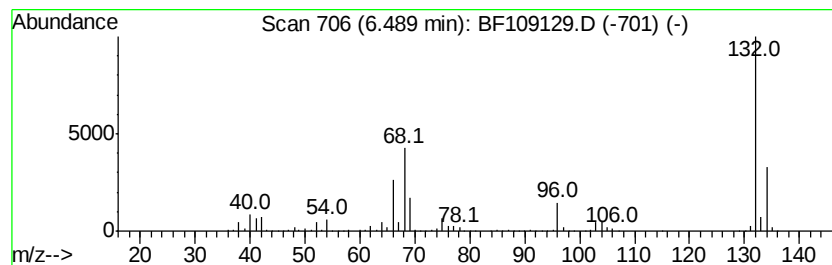
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Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	52.02 ng	2087020	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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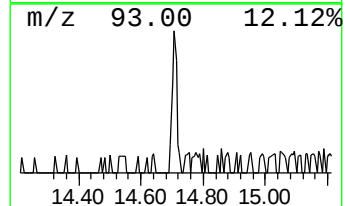
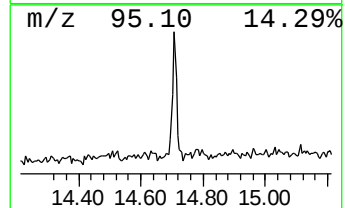
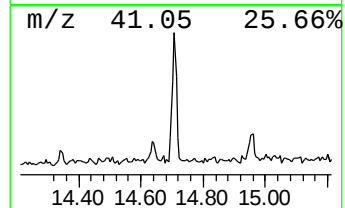
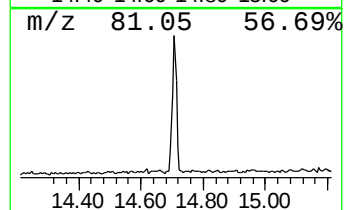
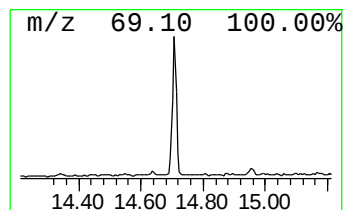
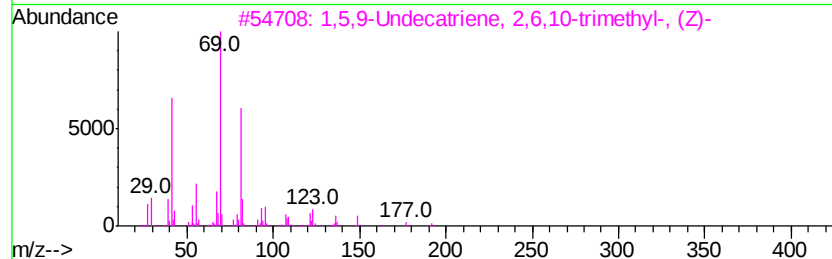
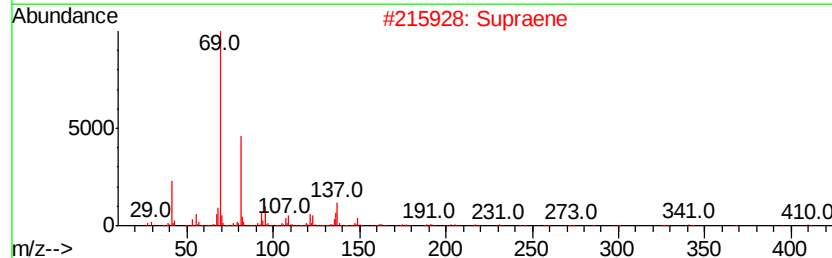
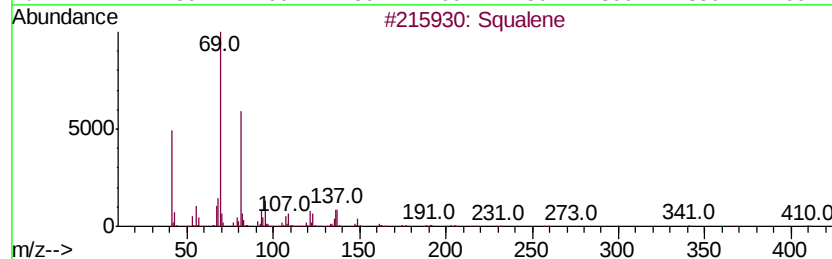
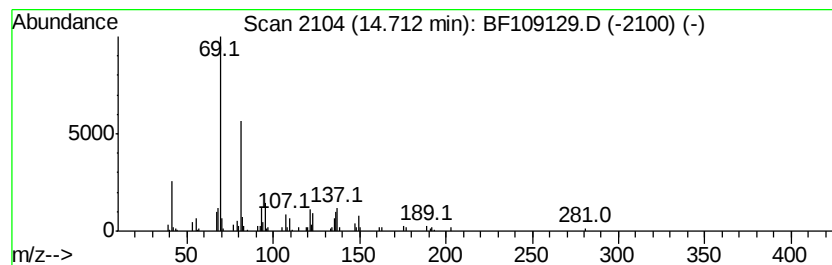
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Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.51 ng	101617	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	3.8	ng	151348	1	6.72	802354	20.0
unknown6.49	6.49	52.0	ng	2087020	1	6.72	802354	20.0
Squalene	14.71	2.5	ng	101617	6	15.26	808267	20.0